

2 Elektronen in 2 verschiedenen räumlichen Orbitalen

Gleiche
Spinfunkt.:

$$\begin{aligned}\Psi_1(1,2) &= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\alpha(1) & \psi_a(2)\alpha(2) \\ \psi_b(1)\alpha(1) & \psi_b(2)\alpha(2) \end{vmatrix} \\ &= \frac{\alpha(1)\alpha(2)}{\sqrt{2}} \begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_b(1) & \psi_b(2) \end{vmatrix}\end{aligned}$$

$$\Rightarrow \hat{s}_z \Psi_1(1,2) = \hbar \Psi_1(1,2)$$

Triplet ($M_S = 1$)

und analog mit $\beta(1)\beta(2)$: $\hat{s}_z \Psi_{-1}(1,2) = -\hbar \Psi_{-1}(1,2)$.

" ($M_S = -1$)

Verschiedene Spinfunktionen:

$$\Psi_0(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\alpha(1) & \psi_a(2)\alpha(2) \\ \psi_b(1)\beta(1) & \psi_b(2)\beta(2) \end{vmatrix}, \quad \hat{s}_z \Psi_0(1,2) = 0$$

$$\Psi'_0(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(1)\beta(1) & \psi_a(2)\beta(2) \\ \psi_b(1)\alpha(1) & \psi_b(2)\alpha(2) \end{vmatrix}, \quad \hat{s}_z \Psi'_0(1,2) = 0$$

$$\begin{aligned}\Rightarrow \frac{1}{\sqrt{2}} [\Psi_0(1,2) \pm \Psi'_0(1,2)] &= \frac{1}{2} [\psi_a(1)\alpha(1)\psi_b(2)\beta(2) - \psi_a(2)\alpha(2)\psi_b(1)\beta(1) \\ &\quad \pm \psi_a(1)\beta(1)\psi_b(2)\alpha(2) \mp \psi_b(1)\alpha(1)\psi_a(2)\beta(2)]\end{aligned}$$

Triplet ($M_S = 0$)

$$= \frac{1}{2} [\psi_a(1)\psi_b(2) \mp \psi_a(2)\psi_b(1)] [\alpha(1)\beta(2) \pm \alpha(2)\beta(1)].$$

Singulett ($M_S = 0$)